Sulfamethoxypyridazine 80-35-3 | DTXSID5023611

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 1.64

Global applicability domain: Inside

Local applicability domain index: 5.61e-01

Confidence level: 5.64e-01

Nearest Neighbors from the Training Set

Image not found

Sulfamethoxypyridazine

Measured: 0.32 Predicted: 1.64

Image not found

2,4-Pyrimidinediamine, 5-(1,3-benzodioxol-5-ylmethyl)-

Measured: 1.51 Predicted: 5.02e-01